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Canada Centre for Mineral and Energy Technology | Centre canadien de la technologie des minéraux et de l'énergie

# THERMODYNAMICS OF COAL CONVERSION REACTIONS

## PART 1. THE WATER - GAS REACTION

R.A. CAMPBELL

COAL CONVERSION SECTION

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# Thermodynamics of Coal Conversion Reactions

## Part 1. The "Water-Gas" Reaction

### INTRODUCTION

The water-gas reaction has long been used in the making of producer gas, a low - BTU gas used for domestic heating, etc., but it has not been widely used in recent years because of the availability of the more convenient forms of fuel. In this process, air and steam are blown upward through a vessel containing coke. The combustion of the fuel by the oxygen of the air raises the temperature, but produces a mixture of CO and $CO_2$, the proportions of which are controlled by the Boudard reaction:

$$C + CO_2 \rightarrow 2CO$$

When steam is added to the input gas the water gas reaction proceeds as follows:

$$C \quad H_2O \rightarrow CO + H_2$$

This reaction is endothermic and causes cooling of the bed. If too much steam is used the bed cools to the point where it becomes inoperative.

This present report is a brief examination of the thermodynamics of the water-gas reaction as a function of temperature. Thermodynamic data for this study were taken from Ref. (1) mainly because these are believed to be reliable data, and they are set forth in a form which is particularly convenient

to use. For each substance of interest, the free energy, $\Delta F$, is set forth as a polynomial function of temperature, in $^{o}K$. Obtaining the equation for the free energy change for a reaction is a simple matter of addition and subtraction of the appropriate terms.

## RESULTS

For the water gas reaction:

$$\underset{(s)}{C} + \underset{(g)}{H_2O} \rightarrow \underset{(g)}{CO} + \underset{(g)}{H_2}$$

$$\Delta F = 31560 - 2.02\ T\ln T + 0.91 \times 10^{-3}\ T^2 - 1.02 \times 10^{5}/T - 20.73T$$

A program was written for the NOVA minicomputer and values for the above equation were calculated from $100^{o}C$ to $1400^{o}C$ in $5^{o}$ intervals. In view of the slight uncertainty present in all thermodynamic data there seemed to be little point in calculating values at every degree.

It was found that for this reaction $\Delta F$ was positive, and K, the equilibrium constant was less than one, up to about $660^{o}C$. Above $660^{o}C$ $\Delta F$ was negative and the equilibrium constant was greater than one. The equilibrium constant was calculated from the relationship:

$$\Delta F = -RT \ln K$$

$$\text{i.e. } K = \text{EXP } \frac{(-\Delta F)}{RT}$$

where R = gas content (1.98647).

The information derived by this calculation is listed in Appendix A.

The above results indicate that in order for the water-gas reaction to play a significant role in the process, a reasonably high temperature e.g. 800 to 1000°C would be advantageous.

Information converning the amount of heat needed to bring the carbon up to operating temperature, and the heat of reaction of the water-gas reaction are also of some interest. An equation were set up to calculate the amount of heat needed to heat the carbon, as follows:

$$H = -1972 + 4.1\ T + 0.0005\ 1\ T^2 + 210000/T$$

The derived answers were expressed in kcal/kg-mol of carbon, and in BTU/lb carbon. For the heat of reaction the derived equation was:

$$HR = 31554 + 2.04\ T - 0.00091\ T^2 - 203000/T$$

In this case the derived answers were expressed only in kcal/kg-mol of carbon. These results are listed in Appendix B.

The heat needed to bring the carbon up to temperature varied from 191 kcal/kg-mol (29 BTU/lb) at 100°C to 6440 kcal/kg-mol (996 BTU/lb) at 1400°C.

The heat of reaction varied very little over the temperature range, from 31644 kcal/kg-mol of carbon at 100°C to 32299 kcal/kg-mol at 1400°C.

## REFERENCES

1. Wicks, C.E. and Block, F.E. "Thermodynamic Properties of 65 Elements - Their Oxides, Halides, Carbides and Nitrides" U.S.B.M. Bull 605. U.S. Government Printing Office, 1963.

# APPENDIX A

## Water-gas Reaction

| TEMP. DEG.C | TEMP. DEG.K | FREE ENERGY KCAL/KG-MOL | LN K | K |
|---|---|---|---|---|
| 100. | 373. | 19219. | -25.94 | 0.543336E-11 |
| 105. | 378. | 19053. | -25.37 | 0.955937E-11 |
| 110. | 383. | 18886. | -24.82 | 0.165763E-10 |
| 115. | 388. | 18719. | -24.29 | 0.283453E-10 |
| 120. | 393. | 18552. | -23.76 | 0.478240E-10 |
| 125. | 398. | 18384. | -23.25 | 0.796512E-10 |
| 130. | 403. | 18217. | -22.76 | 0.131018E -9 |
| 135. | 408. | 18049. | -22.27 | 0.212939E -9 |
| 140. | 413. | 17882. | -21.80 | 0.342100E -9 |
| 145. | 418. | 17714. | -21.33 | 0.543507E -9 |
| 150. | 423. | 17546. | -20.88 | 0.854237E -9 |
| 155. | 428. | 17377. | -20.44 | 0.132873E -8 |
| 160. | 433. | 17209. | -20.01 | 0.204612E -8 |
| 165. | 438. | 17041. | -19.59 | 0.312041E -8 |
| 170. | 443. | 16872. | -19.17 | 0.471434E -8 |
| 175. | 448. | 16703. | -18.77 | 0.705815E -8 |
| 180. | 453. | 16534. | -18.37 | 0.134750E -7 |
| 185. | 458. | 16365. | -17.99 | 0.154145E -7 |
| 190. | 463. | 16196. | -17.61 | 0.224976E -7 |
| 195. | 468. | 16027. | -17.24 | 0.325754E -7 |
| 200. | 473. | 15858. | -16.88 | 0.468053E -7 |
| 205. | 478. | 15688. | -16.52 | 0.667509E -7 |
| 210. | 483. | 15519. | -16.17 | 0.945097E -7 |
| 215. | 488. | 15349. | -15.83 | 0.132877E -6 |
| 220. | 493. | 15180. | -15.50 | 0.185551E -6 |
| 225. | 498. | 15010. | -15.17 | 0.257401E -6 |
| 230. | 503. | 14840. | -14.85 | 0.354791E -6 |
| 235. | 508. | 14670. | -14.54 | 0.485997E -6 |
| 240. | 513. | 14500. | -14.23 | 0.661713E -6 |
| 245. | 518. | 14329. | -13.93 | 0.895688E -6 |
| 250. | 523. | 14159. | -13.63 | 0.120550E -5 |
| 255. | 528. | 13989. | -13.34 | 0.161351E -5 |
| 260. | 533. | 13818. | -13.05 | 0.214799E -5 |
| 265. | 538. | 13648. | -12.77 | 0.284457E -5 |
| 270. | 543. | 13477. | -12.49 | 0.374791E -5 |
| 275. | 548. | 13306. | -12.22 | 0.491369E -5 |
| 280. | 553. | 13136. | -11.96 | 0.641106E -5 |
| 285. | 558. | 12965. | -11.70 | 0.832553E -5 |
| 290. | 563. | 12794. | -11.44 | 0.107623E -4 |
| 295. | 568. | 12623. | -11.19 | 0.138535E -4 |
| 300. | 573. | 12452. | -10.94 | 0.177477E -4 |
| 305. | 578. | 12280. | -10.70 | 0.226454E -4 |
| 310. | 583. | 12109. | -10.46 | 0.287759E -4 |
| 315. | 588. | 11938. | -10.22 | 0.364194E -4 |
| 320. | 593. | 11767. | -9.99 | 0.459129E -4 |
| 325. | 598. | 11595. | -9.76 | 0.576606E -4 |
| 330. | 603. | 11424. | -9.54 | 0.721447E -4 |
| 335. | 608. | 11252. | -9.32 | 0.899398E -4 |
| 340. | 613. | 11080. | -9.10 | 0.111727E -3 |
| 345. | 618. | 10909. | -8.89 | 0.138313E -3 |

| TEMP. DEG.C | TEMP. DEG.K | FREE ENERGY KCAL/KG-MOL | LN K | K |
|---|---|---|---|---|
| 350. | 623. | 10737. | -8.68 | 0.170647E -3 |
| 355. | 628. | 10565. | -8.47 | 0.209846E -3 |
| 360. | 633. | 10393. | -8.27 | 0.257219E -3 |
| 365. | 638. | 10222. | -8.07 | 0.314296E -3 |
| 370. | 643. | 10050. | -7.87 | 0.382860E -3 |
| 375. | 648. | 9878. | -7.67 | 0.464981E -3 |
| 380. | 653. | 9706. | -7.48 | 0.563061E -3 |
| 385. | 658. | 9533. | -7.29 | 0.679876E -3 |
| 390. | 663. | 9361. | -7.11 | 0.818624E -3 |
| 395. | 668. | 9189. | -6.92 | 0.982988E -3 |
| 400. | 673. | 9017. | -6.74 | 0.117719E -2 |
| 405. | 678. | 8845. | -6.57 | 0.140606E -2 |
| 410. | 683. | 8672. | -6.39 | 0.167513E -2 |
| 415. | 688. | 8500. | -6.22 | 0.199067E -2 |
| 420. | 693. | 8327. | -6.05 | 0.235984E -2 |
| 425. | 698. | 8155. | -5.88 | 0.279076E -2 |
| 430. | 703. | 7982. | -5.72 | 0.329259E -2 |
| 435. | 708. | 7810. | -5.55 | 0.387572E -2 |
| 440. | 713. | 7637. | -5.39 | 0.455182E -2 |
| 445. | 718. | 7465. | -5.23 | 0.533405E -2 |
| 450. | 723. | 7292. | -5.08 | 0.623719E -2 |
| 455. | 728. | 7119. | -4.92 | 0.727778E -2 |
| 460. | 733. | 6947. | -4.77 | 0.847433E -2 |
| 465. | 738. | 6774. | -4.62 | 0.984753E -2 |
| 470. | 743. | 6601. | -4.47 | 0.114204E -1 |
| 475. | 748. | 6428. | -4.33 | 0.132186E -1 |
| 480. | 753. | 6255. | -4.18 | 0.152706E -1 |
| 485. | 758. | 6082. | -4.04 | 0.176080E -1 |
| 490. | 763. | 5909. | -3.90 | 0.202558E -1 |
| 495. | 768. | 5736. | -3.76 | 0.232825E -1 |
| 500. | 773. | 5563. | -3.62 | 0.267009E -1 |
| 505. | 778. | 5390. | -3.49 | 0.305579E -1 |
| 510. | 783. | 5217. | -3.35 | 0.349353E -1 |
| 515. | 788. | 5044. | -3.22 | 0.398598E -1 |
| 520. | 793. | 4871. | -3.09 | 0.454036E -1 |
| 525. | 798. | 4698. | -2.96 | 0.516352E -1 |
| 530. | 803. | 4525. | -2.84 | 0.586290E -1 |
| 535. | 808. | 4351. | -2.71 | 0.664668E -1 |
| 540. | 813. | 4178. | -2.59 | 0.752375E -1 |
| 545. | 818. | 4005. | -2.46 | 0.850376E -1 |
| 550. | 823. | 3832. | -2.34 | 0.959731E -1 |
| 555. | 828. | 3658. | -2.22 | 0.108158E 0 |
| 560. | 833. | 3485. | -2.11 | 0.121718E 0 |
| 565. | 838. | 3312. | -1.99 | 0.136786E 0 |
| 570. | 843. | 3138. | -1.87 | 0.153509E 0 |
| 575. | 848. | 2965. | -1.76 | 0.172045E 0 |
| 580. | 853. | 2791. | -1.65 | 0.192564E 0 |
| 585. | 858. | 2618. | -1.54 | 0.215250E 0 |
| 590. | 863. | 2444. | -1.43 | 0.240302E 0 |
| 595. | 868. | 2271. | -1.32 | 0.267932E 0 |

| TEMP. DEG.C | TEMP. DEG.K | FREE ENERGY KCAL/KG-MOL | LN K | K |
|---|---|---|---|---|
| 600. | 873. | 2097. | -1.21 | 0.298371E 0 |
| 605. | 878. | 1924. | -1.10 | 0.331854E 0 |
| 610. | 883. | 1750. | -1.00 | 0.368577E 0 |
| 615. | 888. | 1577. | -0.89 | 0.409093E 0 |
| 620. | 893. | 1403. | -0.79 | 0.453416E 0 |
| 625. | 898. | 1229. | -0.69 | 0.501971E 0 |
| 630. | 903. | 1055. | -0.59 | 0.555105E 0 |
| 635. | 908. | 882. | -0.49 | 0.613189E 0 |
| 640. | 913. | 708. | -0.39 | 0.676620E 0 |
| 645. | 918. | 535. | -0.29 | 0.745819E 0 |
| 650. | 923. | 361. | -0.20 | 0.821235E 0 |
| 655. | 928. | 187. | -0.10 | 0.903347E 0 |
| 660. | 933. | 14. | -0.00 | 0.992563E 0 |
| 665. | 938. | -160. | 0.08 | 0.108972E 1 |
| 670. | 943. | -334. | 0.18 | 0.119510E 1 |
| 675. | 948. | -508. | 0.27 | 0.130940E 1 |
| 680. | 953. | -681. | 0.36 | 0.143327E 1 |
| 685. | 958. | -855. | 0.45 | 0.155738E 1 |
| 690. | 963. | -1029. | 0.54 | 0.171247E 1 |
| 695. | 968. | -1203. | 0.63 | 0.186929E 1 |
| 700. | 973. | -1377. | 0.71 | 0.203854E 1 |
| 705. | 978. | -1551. | 0.80 | 0.222139E 1 |
| 710. | 983. | -1724. | 0.88 | 0.241841E 1 |
| 715. | 988. | -1898. | 0.97 | 0.263056E 1 |
| 720. | 993. | -2072. | 1.05 | 0.285914E 1 |
| 725. | 998. | -2245. | 1.13 | 0.310488E 1 |
| 730. | 1003. | -2420. | 1.21 | 0.336898E 1 |
| 735. | 1008. | -2594. | 1.30 | 0.365262E 1 |
| 740. | 1013. | -2768. | 1.38 | 0.395699E 1 |
| 745. | 1018. | -2942. | 1.45 | 0.428337E 1 |
| 750. | 1023. | -3116. | 1.53 | 0.463310E 1 |
| 755. | 1028. | -3290. | 1.61 | 0.500759E 1 |
| 760. | 1033. | -3464. | 1.69 | 0.540830E 1 |
| 765. | 1038. | -3638. | 1.76 | 0.583676E 1 |
| 770. | 1043. | -3812. | 1.84 | 0.629459E 1 |
| 775. | 1048. | -3986. | 1.91 | 0.678346E 1 |
| 780. | 1053. | -4160. | 1.99 | 0.730514E 1 |
| 785. | 1058. | -4334. | 2.06 | 0.786145E 1 |
| 790. | 1063. | -4508. | 2.13 | 0.845432E 1 |
| 795. | 1068. | -4682. | 2.21 | 0.908574E 1 |
| 800. | 1073. | -4856. | 2.28 | 0.975779E 1 |
| 805. | 1078. | -5030. | 2.35 | 0.104726E 2 |
| 810. | 1083. | -5204. | 2.42 | 0.112326E 2 |
| 815. | 1088. | -5378. | 2.49 | 0.120399E 2 |
| 820. | 1093. | -5552. | 2.56 | 0.128971E 2 |
| 825. | 1098. | -5725. | 2.63 | 0.138067E 2 |
| 830. | 1103. | -5900. | 2.69 | 0.147713E 2 |
| 835. | 1108. | -6074. | 2.76 | 0.157938E 2 |
| 840. | 1113. | -6248. | 2.83 | 0.168769E 2 |
| 845. | 1118. | -6422. | 2.89 | 0.180236E 2 |

| TEMP. DEG.C | TEMP. DEG.K | FREE ENERGY KCAL/KG-MOL | LN K | K |
|---|---|---|---|---|
| 850. | 1123. | -6596. | 2.96 | 0.192370E 2 |
| 855. | 1128. | -5770. | 3.02 | 0.205202E 2 |
| 860. | 1133. | -6944. | 3.09 | 0.218767E 2 |
| 865. | 1138. | -7118. | 3.15 | 0.233096E 2 |
| 870. | 1143. | -7292. | 3.21 | 0.248227E 2 |
| 875. | 1148. | -7466. | 3.27 | 0.264196E 2 |
| 880. | 1153. | -7641. | 3.34 | 0.281040E 2 |
| 885. | 1158. | -7815. | 3.40 | 0.298798E 2 |
| 890. | 1163. | -7989. | 3.46 | 0.317512E 2 |
| 895. | 1168. | -8163. | 3.52 | 0.337222E 2 |
| 900. | 1173. | -8337. | 3.58 | 0.357972E 2 |
| 905. | 1178. | -8511. | 3.64 | 0.379807E 2 |
| 910. | 1183. | -8685. | 3.70 | 0.402772E 2 |
| 915. | 1188. | -8859. | 3.75 | 0.426914E 2 |
| 920. | 1193. | -9033. | 3.81 | 0.452283E 2 |
| 925. | 1198. | -9207. | 3.87 | 0.478929E 2 |
| 930. | 1203. | -9381. | 3.93 | 0.506902E 2 |
| 935. | 1208. | -9555. | 3.98 | 0.535258E 2 |
| 940. | 1213. | -9730. | 4.04 | 0.565050E 2 |
| 945. | 1218. | -9904. | 4.09 | 0.596336E 2 |
| 950. | 1223. | -10078. | 4.15 | 0.629172E 2 |
| 955. | 1228. | -10252. | 4.20 | 0.663619E 2 |
| 960. | 1233. | -10426. | 4.26 | 0.699739E 2 |
| 965. | 1238. | -10600. | 4.31 | 0.737593E 2 |
| 970. | 1243. | -10774. | 4.36 | 0.777247E 2 |
| 975. | 1248. | -10948. | 4.42 | 0.818768E 2 |
| 980. | 1253. | -11122. | 4.47 | 0.862223E 2 |
| 985. | 1258. | -11296. | 4.52 | 0.907684E 2 |
| 990. | 1263. | -11470. | 4.57 | 0.955218E 2 |
| 995. | 1268. | -11644. | 4.62 | 0.101790E 3 |
| 1000. | 1273. | -11818. | 4.67 | 0.107081E 3 |
| 1005. | 1278. | -11993. | 4.72 | 0.112603E 3 |
| 1010. | 1283. | -12167. | 4.77 | 0.118362E 3 |
| 1015. | 1288. | -12341. | 4.82 | 0.124358E 3 |
| 1020. | 1293. | -12515. | 4.87 | 0.130628E 3 |
| 1025. | 1298. | -12689. | 4.92 | 0.137151E 3 |
| 1030. | 1303. | -12863. | 4.97 | 0.143946E 3 |
| 1035. | 1308. | -13037. | 5.02 | 0.151021E 3 |
| 1040. | 1313. | -13211. | 5.07 | 0.158386E 3 |
| 1045. | 1318. | -13385. | 5.11 | 0.166050E 3 |
| 1050. | 1323. | -13559. | 5.16 | 0.174022E 3 |
| 1055. | 1328. | -13733. | 5.21 | 0.182312E 3 |
| 1060. | 1333. | -13907. | 5.25 | 0.190930E 3 |
| 1065. | 1338. | -14081. | 5.30 | 0.199885E 3 |
| 1070. | 1343. | -14255. | 5.34 | 0.209189E 3 |
| 1075. | 1348. | -14429. | 5.39 | 0.218852E 3 |
| 1080. | 1353. | -14603. | 5.43 | 0.228885E 3 |
| 1085. | 1358. | -14777. | 5.48 | 0.239297E 3 |
| 1090. | 1363. | -14951. | 5.52 | 0.250102E 3 |
| 1095. | 1368. | -15125. | 5.57 | 0.261308E 3 |

| TEMP. DEG.C | TEMP. DEG.K | FREE ENERGY KCAL/KG-MOL | LN K | K |
|---|---|---|---|---|
| 1100. | 1373. | -15299. | 5.51 | 0.272930E 3 |
| 1105. | 1378. | -15473. | 5.65 | 0.284977E 3 |
| 1110. | 1383. | -15547. | 5.70 | 0.297463E 3 |
| 1115. | 1388. | -15821. | 5.74 | 0.310399E 3 |
| 1120. | 1393. | -15994. | 5.78 | 0.323797E 3 |
| 1125. | 1398. | -16168. | 5.82 | 0.337671E 3 |
| 1130. | 1403. | -16342. | 5.86 | 0.352033E 3 |
| 1135. | 1408. | -16516. | 5.91 | 0.366897E 3 |
| 1140. | 1413. | -16690. | 5.95 | 0.382275E 3 |
| 1145. | 1418. | -16864. | 5.99 | 0.398181E 3 |
| 1150. | 1423. | -17038. | 6.03 | 0.414630E 3 |
| 1155. | 1428. | -17212. | 6.07 | 0.431633E 3 |
| 1160. | 1433. | -17386. | 6.11 | 0.449207E 3 |
| 1165. | 1438. | -17559. | 6.15 | 0.467366E 3 |
| 1170. | 1443. | -17733. | 6.19 | 0.486123E 3 |
| 1175. | 1448. | -17907. | 6.23 | 0.505494E 3 |
| 1180. | 1453. | -18081. | 6.26 | 0.525494E 3 |
| 1185. | 1458. | -18255. | 6.30 | 0.546139E 3 |
| 1190. | 1463. | -18429. | 6.34 | 0.567443E 3 |
| 1195. | 1468. | -18602. | 6.38 | 0.589423E 3 |
| 1200. | 1473. | -18776. | 6.42 | 0.612094E 3 |
| 1205. | 1478. | -18950. | 6.45 | 0.635473E 3 |
| 1210. | 1483. | -19124. | 6.49 | 0.659575E 3 |
| 1215. | 1488. | -19298. | 6.53 | 0.684419E 3 |
| 1220. | 1493. | -19471. | 6.57 | 0.710020E 3 |
| 1225. | 1498. | -19645. | 6.60 | 0.736395E 3 |
| 1230. | 1503. | -19819. | 6.64 | 0.763563E 3 |
| 1235. | 1508. | -19993. | 6.67 | 0.791539E 3 |
| 1240. | 1513. | -20166. | 6.71 | 0.820343E 3 |
| 1245. | 1518. | -20340. | 6.75 | 0.849992E 3 |
| 1250. | 1523. | -20514. | 6.78 | 0.880503E 3 |
| 1255. | 1528. | -20687. | 6.82 | 0.911897E 3 |
| 1260. | 1533. | -20861. | 6.85 | 0.944190E 3 |
| 1265. | 1538. | -21035. | 6.88 | 0.977403E 3 |
| 1270. | 1543. | -21208. | 6.92 | 0.101155E 4 |
| 1275. | 1548. | -21382. | 6.95 | 0.104566E 4 |
| 1280. | 1553. | -21556. | 6.99 | 0.108274E 4 |
| 1285. | 1558. | -21729. | 7.02 | 0.111982E 4 |
| 1290. | 1563. | -21903. | 7.05 | 0.115792E 4 |
| 1295. | 1568. | -22075. | 7.09 | 0.119705E 4 |
| 1300. | 1573. | -22250. | 7.12 | 0.123724E 4 |
| 1305. | 1578. | -22424. | 7.15 | 0.127850E 4 |
| 1310. | 1583. | -22597. | 7.19 | 0.132087E 4 |
| 1315. | 1588. | -22771. | 7.22 | 0.136435E 4 |
| 1320. | 1593. | -22944. | 7.25 | 0.140897E 4 |
| 1325. | 1598. | -23118. | 7.28 | 0.145475E 4 |
| 1330. | 1603. | -23291. | 7.31 | 0.150171E 4 |
| 1335. | 1608. | -23465. | 7.35 | 0.154988E 4 |
| 1340. | 1613. | -23638. | 7.38 | 0.159927E 4 |
| 1345. | 1618. | -23812. | 7.41 | 0.164991E 4 |

| TEMP. DEG.C | TEMP. DEG.K | FREE ENERGY KCAL/KG-MOL | LN K | K |
|---|---|---|---|---|
| 1350. | 1623. | -23985. | 7.44 | 0.170181E 4 |
| 1355. | 1628. | -24159. | 7.47 | 0.175501E 4 |
| 1360. | 1633. | -24332. | 7.50 | 0.180953E 4 |
| 1365. | 1638. | -24505. | 7.53 | 0.186538E 4 |
| 1370. | 1643. | -24679. | 7.56 | 0.192259E 4 |
| 1375. | 1648. | -24852. | 7.59 | 0.198119E 4 |
| 1380. | 1653. | -25025. | 7.62 | 0.204119E 4 |
| 1385. | 1658. | -25199. | 7.65 | 0.210262E 4 |
| 1390. | 1663. | -25372. | 7.68 | 0.216551E 4 |
| 1395. | 1668. | -25546. | 7.71 | 0.222987E 4 |
| 1400. | 1673. | -25719. | 7.74 | 0.229574E 4 |

```
 A=      31560.000000
 B=         -2.020000
 C=          0.000910
 D=   -102000.000000
 E =       -20.730010

EQUATION: F = A + B*T*LN(T) + C*T *T + D/T + E*T
STOP
R
```

# APPENDIX B

## Water-Gas Reaction

| TEMP. DEG.C | TEMP. DEG.K | TO HEAT CARBON KCAL/KG-MOL | BTU/LB | HEAT OF REACTION KCAL/KG-MOL |
|---|---|---|---|---|
| 100. | 373. | 191. | 29. | 31644. |
| 105. | 378. | 206. | 31. | 31658. |
| 110. | 383. | 221. | 33. | 31672. |
| 115. | 388. | 237. | 35. | 31685. |
| 120. | 393. | 252. | 38. | 31699. |
| 125. | 398. | 268. | 40. | 31712. |
| 130. | 403. | 284. | 43. | 31725. |
| 135. | 408. | 300. | 45. | 31737. |
| 140. | 413. | 317. | 48. | 31750. |
| 145. | 418. | 333. | 50. | 31762. |
| 150. | 423. | 350. | 52. | 31774. |
| 155. | 428. | 367. | 55. | 31786. |
| 160. | 433. | 384. | 58. | 31798. |
| 165. | 438. | 401. | 60. | 31809. |
| 170. | 443. | 418. | 63. | 31821. |
| 175. | 448. | 436. | 65. | 31832. |
| 180. | 453. | 454. | 68. | 31843. |
| 185. | 458. | 471. | 71. | 31854. |
| 190. | 463. | 489. | 73. | 31865. |
| 195. | 468. | 507. | 76. | 31876. |
| 200. | 473. | 525. | 79. | 31886. |
| 205. | 478. | 544. | 82. | 31897. |
| 210. | 483. | 562. | 84. | 31907. |
| 215. | 488. | 581. | 87. | 31917. |
| 220. | 493. | 599. | 90. | 31927. |
| 225. | 498. | 618. | 93. | 31937. |
| 230. | 503. | 637. | 96. | 31946. |
| 235. | 508. | 656. | 98. | 31956. |
| 240. | 513. | 675. | 101. | 31965. |
| 245. | 518. | 694. | 104. | 31975. |
| 250. | 523. | 713. | 107. | 31984. |
| 255. | 528. | 733. | 110. | 31993. |
| 260. | 533. | 752. | 113. | 32002. |
| 265. | 538. | 772. | 116. | 32011. |
| 270. | 543. | 791. | 119. | 32020. |
| 275. | 548. | 811. | 122. | 32028. |
| 280. | 553. | 831. | 125. | 32037. |
| 285. | 558. | 851. | 128. | 32045. |
| 290. | 563. | 871. | 131. | 32054. |
| 295. | 568. | 891. | 134. | 32062. |
| 300. | 573. | 911. | 137. | 32070. |
| 305. | 578. | 932. | 140. | 32078. |
| 310. | 583. | 952. | 143. | 32086. |
| 315. | 588. | 972. | 146. | 32094. |
| 320. | 593. | 993. | 149. | 32101. |
| 325. | 598. | 1013. | 152. | 32109. |
| 330. | 603. | 1034. | 155. | 32117. |
| 335. | 608. | 1055. | 158. | 32124. |
| 340. | 613. | 1076. | 161. | 32131. |
| 345. | 618. | 1096. | 164. | 32139. |

| TEMP. DEG.C | TEMP. DEG.K | TO HEAT CARBON KCAL/KG-MOL | TO HEAT CARBON BTU/LB | HEAT OF REACTION KCAL/KG-MOL |
|---|---|---|---|---|
| 350. | 623. | 1117. | 168. | 32146. |
| 355. | 628. | 1138. | 171. | 32153. |
| 360. | 633. | 1159. | 174. | 32160. |
| 365. | 638. | 1181. | 177. | 32167. |
| 370. | 643. | 1202. | 180. | 32174. |
| 375. | 648. | 1223. | 183. | 32181. |
| 380. | 653. | 1244. | 187. | 32187. |
| 385. | 658. | 1266. | 190. | 32194. |
| 390. | 663. | 1287. | 193. | 32200. |
| 395. | 668. | 1309. | 196. | 32207. |
| 400. | 673. | 1330. | 200. | 32213. |
| 405. | 678. | 1352. | 203. | 32219. |
| 410. | 683. | 1374. | 206. | 32226. |
| 415. | 688. | 1395. | 209. | 32232. |
| 420. | 693. | 1417. | 213. | 32238. |
| 425. | 698. | 1439. | 216. | 32244. |
| 430. | 703. | 1461. | 219. | 32250. |
| 435. | 708. | 1483. | 222. | 32255. |
| 440. | 713. | 1505. | 226. | 32261. |
| 445. | 718. | 1527. | 229. | 32267. |
| 450. | 723. | 1549. | 232. | 32272. |
| 455. | 728. | 1572. | 236. | 32278. |
| 460. | 733. | 1594. | 239. | 32283. |
| 465. | 738. | 1616. | 242. | 32289. |
| 470. | 743. | 1638. | 246. | 32294. |
| 475. | 748. | 1661. | 249. | 32299. |
| 480. | 753. | 1683. | 252. | 32305. |
| 485. | 758. | 1706. | 256. | 32310. |
| 490. | 763. | 1728. | 259. | 32315. |
| 495. | 768. | 1751. | 263. | 32320. |
| 500. | 773. | 1774. | 266. | 32325. |
| 505. | 778. | 1795. | 269. | 32329. |
| 510. | 783. | 1819. | 273. | 32334. |
| 515. | 788. | 1842. | 276. | 32339. |
| 520. | 793. | 1865. | 280. | 32343. |
| 525. | 798. | 1888. | 283. | 32348. |
| 530. | 803. | 1911. | 287. | 32353. |
| 535. | 808. | 1934. | 290. | 32357. |
| 540. | 813. | 1957. | 293. | 32361. |
| 545. | 818. | 1980. | 297. | 32365. |
| 550. | 823. | 2003. | 300. | 32370. |
| 555. | 828. | 2026. | 304. | 32374. |
| 560. | 833. | 2049. | 307. | 32378. |
| 565. | 838. | 2073. | 311. | 32382. |
| 570. | 843. | 2096. | 314. | 32386. |
| 575. | 848. | 2119. | 318. | 32390. |
| 580. | 853. | 2143. | 321. | 32394. |
| 585. | 858. | 2166. | 325. | 32398. |
| 590. | 863. | 2189. | 328. | 32402. |
| 595. | 868. | 2213. | 332. | 32405. |

| TEMP. DEG.C | TEMP. DEG.K | TO HEAT CARBON KCAL/KG-MOL | BTU/LB | HEAT OF REACTION KCAL/KG-MOL |
|---|---|---|---|---|
| 600. | 873. | 2237. | 335. | 32409. |
| 605. | 878. | 2260. | 339. | 32412. |
| 610. | 883. | 2284. | 343. | 32416. |
| 615. | 888. | 2307. | 346. | 32419. |
| 620. | 893. | 2331. | 350. | 32423. |
| 625. | 898. | 2355. | 353. | 32426. |
| 630. | 903. | 2379. | 357. | 32429. |
| 635. | 908. | 2403. | 360. | 32432. |
| 640. | 913. | 2426. | 364. | 32436. |
| 645. | 918. | 2450. | 368. | 32439. |
| 650. | 923. | 2474. | 371. | 32442. |
| 655. | 928. | 2498. | 375. | 32445. |
| 660. | 933. | 2522. | 378. | 32448. |
| 665. | 938. | 2546. | 382. | 32450. |
| 670. | 943. | 2571. | 386. | 32453. |
| 675. | 948. | 2595. | 389. | 32456. |
| 680. | 953. | 2619. | 393. | 32459. |
| 685. | 958. | 2643. | 396. | 32461. |
| 690. | 963. | 2667. | 400. | 32464. |
| 695. | 968. | 2692. | 404. | 32466. |
| 700. | 973. | 2716. | 407. | 32469. |
| 705. | 978. | 2740. | 411. | 32471. |
| 710. | 983. | 2765. | 415. | 32473. |
| 715. | 988. | 2789. | 418. | 32476. |
| 720. | 993. | 2814. | 422. | 32478. |
| 725. | 998. | 2838. | 425. | 32480. |
| 730. | 1003. | 2863. | 429. | 32482. |
| 735. | 1008. | 2887. | 433. | 32484. |
| 740. | 1013. | 2912. | 437. | 32486. |
| 745. | 1018. | 2937. | 440. | 32488. |
| 750. | 1023. | 2961. | 444. | 32490. |
| 755. | 1028. | 2986. | 448. | 32492. |
| 760. | 1033. | 3011. | 452. | 32494. |
| 765. | 1038. | 3036. | 455. | 32495. |
| 770. | 1043. | 3060. | 459. | 32497. |
| 775. | 1048. | 3085. | 463. | 32499. |
| 780. | 1053. | 3110. | 466. | 32500. |
| 785. | 1058. | 3135. | 470. | 32502. |
| 790. | 1063. | 3160. | 474. | 32503. |
| 795. | 1068. | 3185. | 478. | 32505. |
| 800. | 1073. | 3210. | 481. | 32506. |
| 805. | 1078. | 3235. | 485. | 32507. |
| 810. | 1083. | 3260. | 489. | 32509. |
| 815. | 1088. | 3286. | 493. | 32510. |
| 820. | 1093. | 3311. | 497. | 32511. |
| 825. | 1098. | 3336. | 500. | 32512. |
| 830. | 1103. | 3361. | 504. | 32513. |
| 835. | 1108. | 3386. | 508. | 32514. |
| 840. | 1113. | 3412. | 512. | 32515. |
| 845. | 1118. | 3437. | 515. | 32516. |

| TEMP. DEG.C | TEMP. DEG.K | TO HEAT CARBON KCAL/KG-MOL | BTU/LB | HEAT OF REACTION KCAL/KG-MOL |
|---|---|---|---|---|
| 850. | 1123. | 3462. | 519. | 32517. |
| 855. | 1128. | 3488. | 523. | 32517. |
| 860. | 1133. | 3513. | 527. | 32518. |
| 865. | 1138. | 3539. | 531. | 32519. |
| 870. | 1143. | 3564. | 535. | 32519. |
| 875. | 1148. | 3590. | 538. | 32520. |
| 880. | 1153. | 3615. | 542. | 32520. |
| 885. | 1158. | 3641. | 546. | 32521. |
| 890. | 1163. | 3667. | 550. | 32521. |
| 895. | 1168. | 3692. | 554. | 32521. |
| 900. | 1173. | 3718. | 558. | 32522. |
| 905. | 1178. | 3744. | 561. | 32522. |
| 910. | 1183. | 3770. | 565. | 32522. |
| 915. | 1188. | 3795. | 569. | 32522. |
| 920. | 1193. | 3821. | 573. | 32522. |
| 925. | 1198. | 3847. | 577. | 32522. |
| 930. | 1203. | 3873. | 581. | 32522. |
| 935. | 1208. | 3899. | 585. | 32522. |
| 940. | 1213. | 3925. | 589. | 32522. |
| 945. | 1218. | 3951. | 593. | 32522. |
| 950. | 1223. | 3977. | 596. | 32522. |
| 955. | 1228. | 4003. | 600. | 32522. |
| 960. | 1233. | 4029. | 604. | 32521. |
| 965. | 1238. | 4055. | 608. | 32521. |
| 970. | 1243. | 4081. | 612. | 32520. |
| 975. | 1248. | 4107. | 616. | 32520. |
| 980. | 1253. | 4134. | 620. | 32519. |
| 985. | 1258. | 4160. | 624. | 32519. |
| 990. | 1263. | 4186. | 628. | 32518. |
| 995. | 1268. | 4212. | 632. | 32518. |
| 1000. | 1273. | 4239. | 636. | 32517. |
| 1005. | 1278. | 4265. | 640. | 32516. |
| 1010. | 1283. | 4291. | 644. | 32515. |
| 1015. | 1288. | 4318. | 648. | 32514. |
| 1020. | 1293. | 4344. | 652. | 32513. |
| 1025. | 1298. | 4371. | 655. | 32512. |
| 1030. | 1303. | 4397. | 660. | 32511. |
| 1035. | 1308. | 4424. | 663. | 32510. |
| 1040. | 1313. | 4450. | 667. | 32509. |
| 1045. | 1318. | 4477. | 671. | 32508. |
| 1050. | 1323. | 4504. | 675. | 32507. |
| 1055. | 1328. | 4530. | 679. | 32505. |
| 1060. | 1333. | 4557. | 683. | 32504. |
| 1065. | 1338. | 4584. | 687. | 32503. |
| 1070. | 1343. | 4611. | 691. | 32501. |
| 1075. | 1348. | 4637. | 696. | 32500. |
| 1080. | 1353. | 4664. | 700. | 32498. |
| 1085. | 1358. | 4691. | 704. | 32497. |
| 1090. | 1363. | 4718. | 708. | 32495. |
| 1095. | 1368. | 4745. | 712. | 32493. |

| TEMP. DEG.C | TEMP. DEG.K | TO HEAT CARBON KCAL/KG-MOL | TO HEAT CARBON BTU/LB | HEAT OF REACTION KCAL/KG-MOL |
|---|---|---|---|---|
| 1100. | 1373. | 4772. | 716. | 32492. |
| 1105. | 1378. | 4799. | 720. | 32490. |
| 1110. | 1383. | 4826. | 724. | 32488. |
| 1115. | 1388. | 4853. | 728. | 32486. |
| 1120. | 1393. | 4880. | 732. | 32484. |
| 1125. | 1398. | 4907. | 736. | 32482. |
| 1130. | 1403. | 4934. | 740. | 32480. |
| 1135. | 1408. | 4961. | 744. | 32478. |
| 1140. | 1413. | 4988. | 748. | 32476. |
| 1145. | 1418. | 5015. | 752. | 32474. |
| 1150. | 1423. | 5043. | 756. | 32472. |
| 1155. | 1428. | 5070. | 760. | 32469. |
| 1160. | 1433. | 5097. | 764. | 32467. |
| 1165. | 1438. | 5124. | 769. | 32465. |
| 1170. | 1443. | 5152. | 773. | 32462. |
| 1175. | 1448. | 5179. | 777. | 32460. |
| 1180. | 1453. | 5207. | 781. | 32457. |
| 1185. | 1458. | 5234. | 785. | 32455. |
| 1190. | 1463. | 5261. | 789. | 32452. |
| 1195. | 1468. | 5289. | 793. | 32449. |
| 1200. | 1473. | 5316. | 797. | 32447. |
| 1205. | 1478. | 5344. | 801. | 32444. |
| 1210. | 1483. | 5372. | 806. | 32441. |
| 1215. | 1488. | 5399. | 810. | 32438. |
| 1220. | 1493. | 5427. | 814. | 32435. |
| 1225. | 1498. | 5454. | 818. | 32432. |
| 1230. | 1503. | 5482. | 822. | 32429. |
| 1235. | 1508. | 5510. | 826. | 32426. |
| 1240. | 1513. | 5538. | 831. | 32423. |
| 1245. | 1518. | 5565. | 835. | 32420. |
| 1250. | 1523. | 5593. | 839. | 32417. |
| 1255. | 1528. | 5621. | 843. | 32414. |
| 1260. | 1533. | 5649. | 847. | 32410. |
| 1265. | 1538. | 5677. | 851. | 32407. |
| 1270. | 1543. | 5705. | 856. | 32404. |
| 1275. | 1548. | 5733. | 860. | 32400. |
| 1280. | 1553. | 5761. | 864. | 32397. |
| 1285. | 1558. | 5789. | 868. | 32393. |
| 1290. | 1563. | 5817. | 872. | 32390. |
| 1295. | 1568. | 5845. | 877. | 32386. |
| 1300. | 1573. | 5873. | 881. | 32382. |
| 1305. | 1578. | 5901. | 885. | 32378. |
| 1310. | 1583. | 5929. | 889. | 32375. |
| 1315. | 1588. | 5957. | 893. | 32371. |
| 1320. | 1593. | 5985. | 898. | 32367. |
| 1325. | 1598. | 6014. | 902. | 32363. |
| 1330. | 1603. | 6042. | 906. | 32359. |
| 1335. | 1608. | 6070. | 910. | 32355. |
| 1340. | 1613. | 6098. | 915. | 32351. |
| 1345. | 1618. | 6127. | 919. | 32347. |

| TEMP. DEG.C | TEMP. DEG.K | TO HEAT CARBON KCAL/KG-MOL | TO HEAT CARBON BTU/LB | HEAT OF REACTION KCAL/KG-MOL |
|---|---|---|---|---|
| 1350. | 1623. | 6155. | 923. | 32343. |
| 1355. | 1628. | 6183. | 927. | 32339. |
| 1360. | 1633. | 6212. | 932. | 32334. |
| 1365. | 1638. | 6240. | 936. | 32330. |
| 1370. | 1643. | 6269. | 940. | 32326. |
| 1375. | 1648. | 6297. | 944. | 32321. |
| 1380. | 1653. | 6326. | 949. | 32317. |
| 1385. | 1658. | 6354. | 953. | 32312. |
| 1390. | 1663. | 6383. | 957. | 32308. |
| 1395. | 1668. | 6412. | 962. | 32303. |
| 1400. | 1673. | 6440. | 966. | 32299. |

STOP
R

POOR

QUALITY

ORIGINAL